Dynamical Solutions to the Ground State of a Frustrated Magnet

PHYS 598 Final Presentation

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April 4th, 2025

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What is a Magnet?

- A magnet is a material where the atomic dipoles exhibit some kind of spatial order. Depending on the alignment of the dipoles, a magnetic field may be produced.

- This field is what produces a force that attracts or repulses other ferromagnetic materials, such as iron, nickel, cobalt, etc.

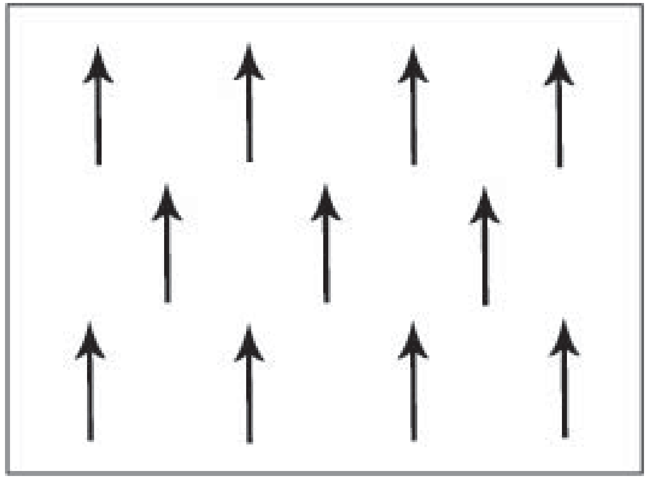


Figure 1: Schematic showing the magnetic dipole moments moments aligned in a ferromagnetic material [1]

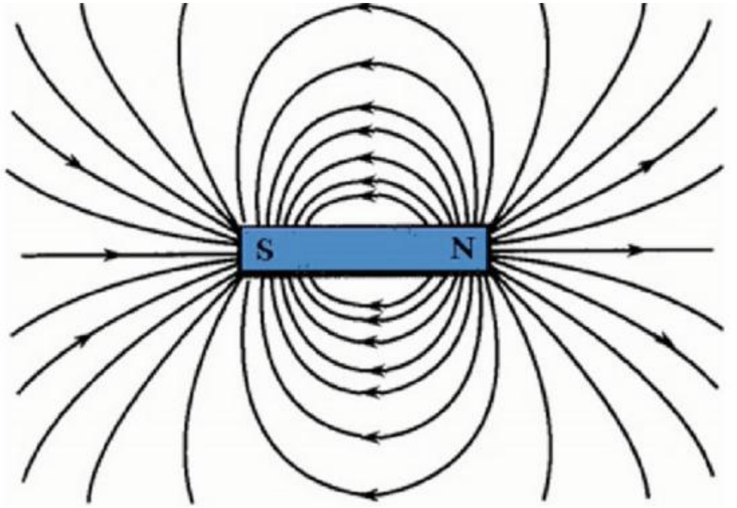
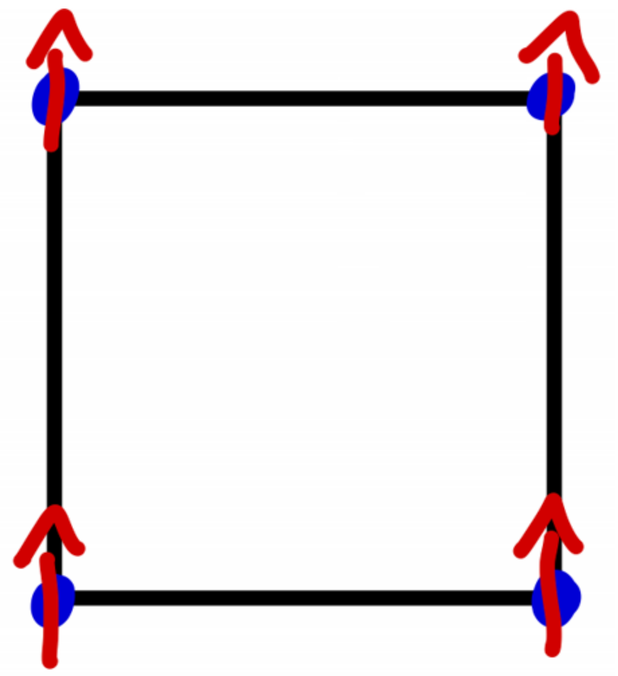


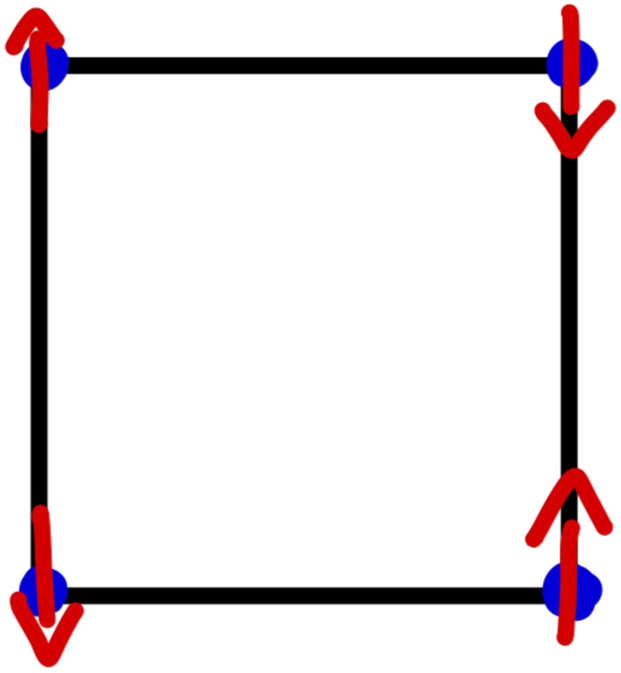
Figure 2: Magnetic field lines of a dipole [2]

Three types of Magnet Dipole Alignment



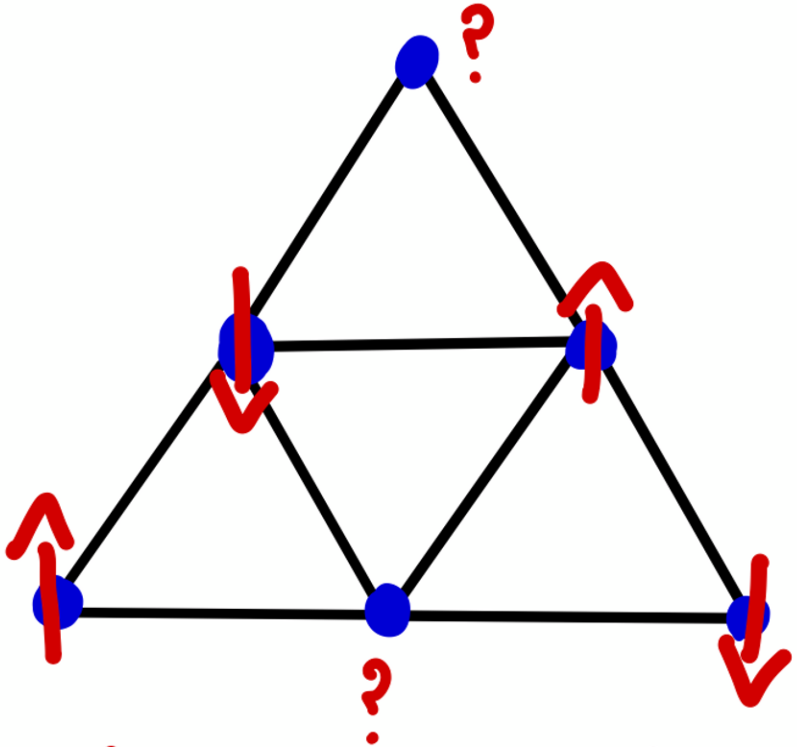
Ferromagnetic

Dipoles aligned in a regular pattern in same direction



Anti Ferromagnetic

Dipoles aligned in a regular pattern in opposite direction



Frustrated Anti Ferromagnetic

Dipoles are not aligned in a regular pattern

Simplified Ising Model

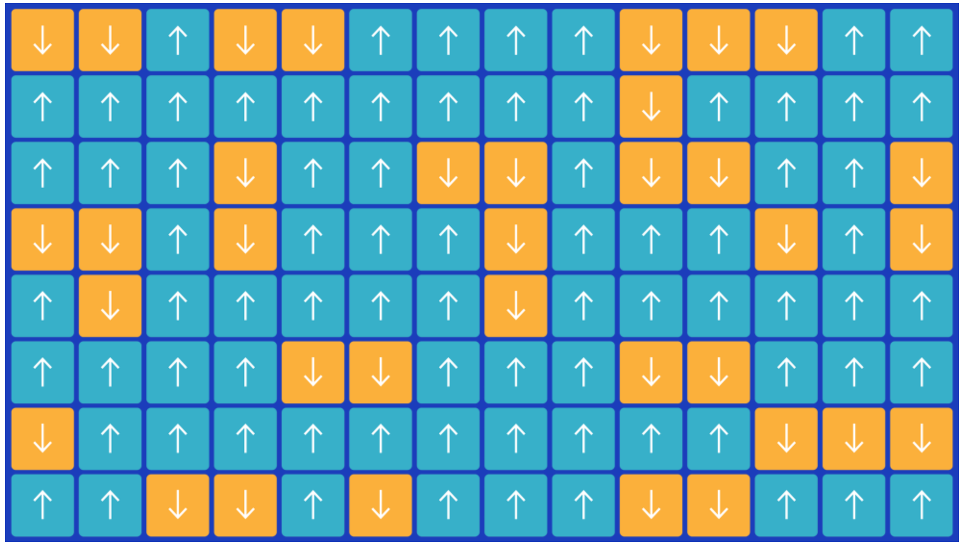


Figure 3: Animation of dipoles being in a superposition of many of different states [3]

- The Simplified Ising Model is used to study how local interactions can give rise to collective behavior in physical systems.

- As seen in the animation, the spins inside the material want to be aligned, but systemic noise creates clumps that prevent this and create frustration.

Using the Ising Model to find the total energy of the system

- The total energy of the system can be found by summing the pairwise interactions, as described by the following Hamiltonian:

$$H(\sigma) = -J \sum_{i,j} \sigma_i \sigma_j$$

- Here, $H(\sigma)$ represents the total energy of the system, J is the coupling constant, and σ_i and σ_j are the spin states of each dipole.
  - $J > 0 \implies$ Lower energy in a *Ferromagnetic* System
  - $J < 0 \implies$ Lower energy in a *Anti Ferromagnetic* System

Creating the Frustrated Ferromagnetic Lattice

- Define a grid of dipoles that is size N x M
- Consider the neighboring interactions: right, down, right-diagonal
- Periodicity at boundaries to simulate a (repeating) infinite system

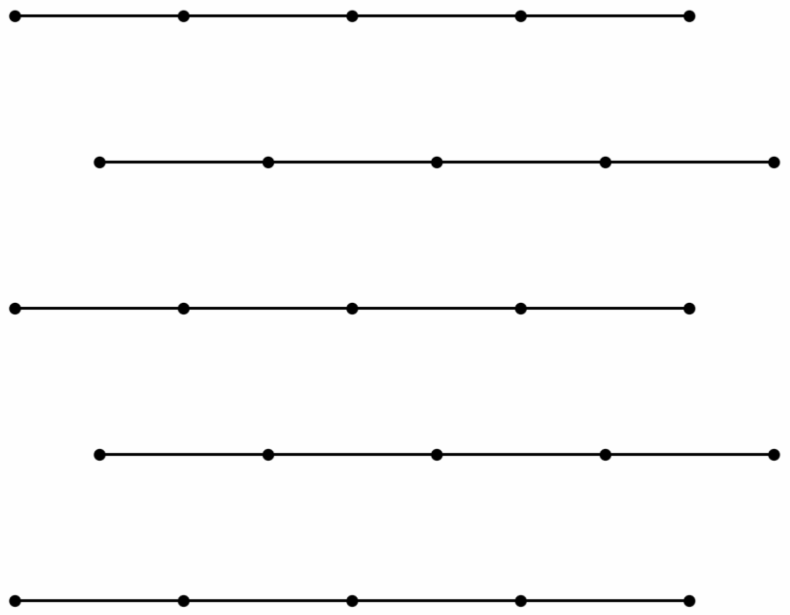
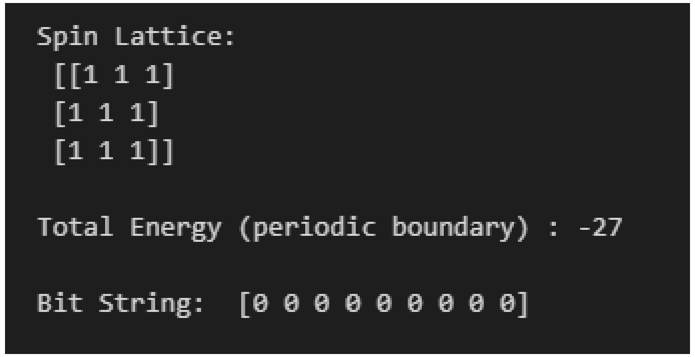


Figure 4: Animation showing a N x M grid turned into a triangular lattice.

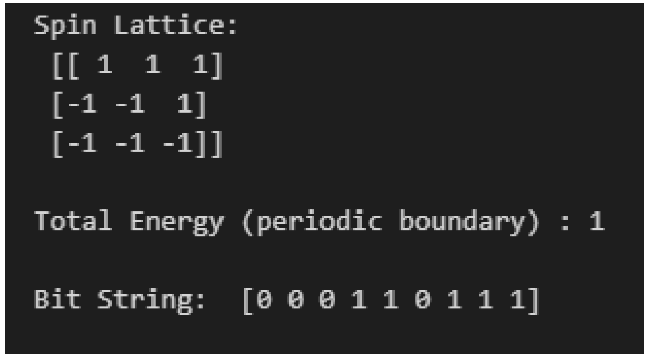
Bitwise Notation and Creating the Lattice

- A N x M grid will have $2^{(N\times M)}$ possible configurations, and we need an efficient method of “bookkeeping” to keep track of each specific configuration.

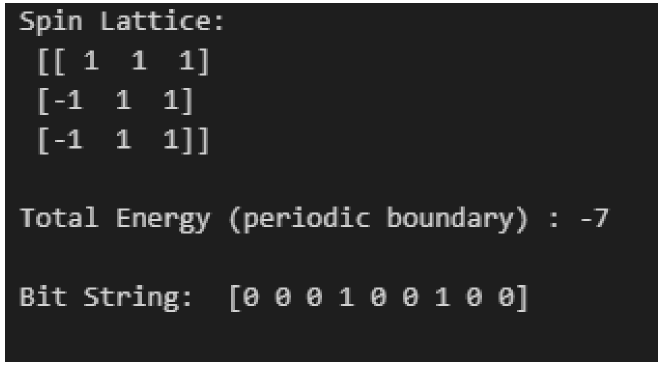
- My approach was to represent each configuration as a bitstring, where each bit corresponds to the spin state of a dipole.



```
Spin Lattice:
 [[1 1 1]
 [1 1 1]
 [1 1 1]]

Total Energy (periodic boundary) : -27

Bit String:  [0 0 0 0 0 0 0 0 0]
```



```
Spin Lattice:
 [[ 1  1  1]
 [-1 -1  1]
 [-1 -1 -1]]

Total Energy (periodic boundary) : 1

Bit String:  [0 0 0 1 1 0 1 1 1]
```

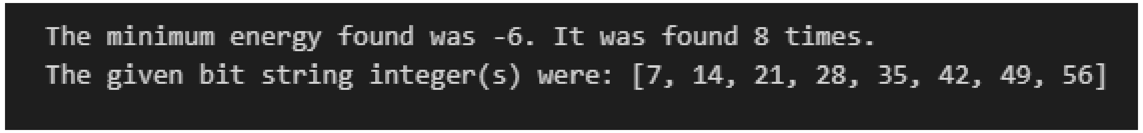


```
Spin Lattice:
 [[ 1  1  1]
 [-1  1  1]
 [-1  1  1]]

Total Energy (periodic boundary) : -7

Bit String:  [0 0 0 1 0 0 1 0 0]
```

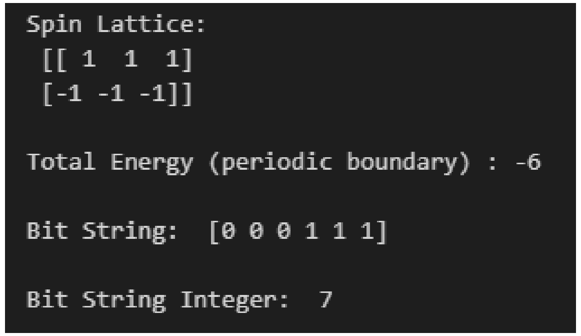
Finding the Superposition of the Ground State

- The ground state is a superposition of all the configurations with the lowest energy. To find these, we need to iterate through all possible configurations and identify those with minimum energy.

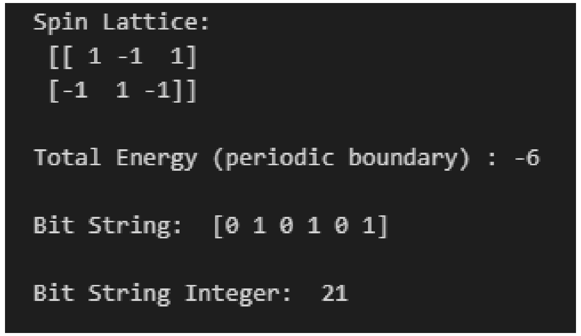
- For example, I found that for a 2×3 lattice, the minimum energy was -6, and occurred 8 times in the $2^{(2\times3)} = 64$ total combinations.



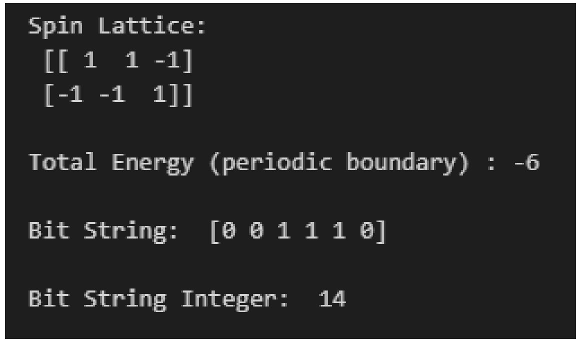
```
The minimum energy found was -6. It was found 8 times.
The given bit string integer(s) were: [7, 14, 21, 28, 35, 42, 49, 56]
```



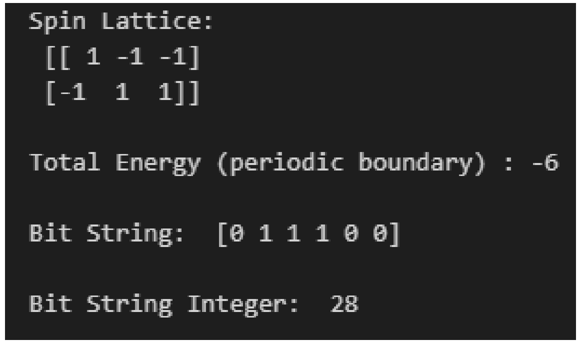
```
Spin Lattice:
 [[ 1  1  1]
 [-1 -1 -1]]

Total Energy (periodic boundary) : -6

Bit String:  [0 0 0 1 1 1]

Bit String Integer:  7
```



```
Spin Lattice:
 [[ 1 -1  1]
 [-1  1 -1]]

Total Energy (periodic boundary) : -6

Bit String:  [0 1 0 1 0 1]

Bit String Integer:  21
```



```
Spin Lattice:
 [[ 1  1 -1]
 [-1 -1  1]]

Total Energy (periodic boundary) : -6

Bit String:  [0 0 1 1 1 0]

Bit String Integer:  14
```

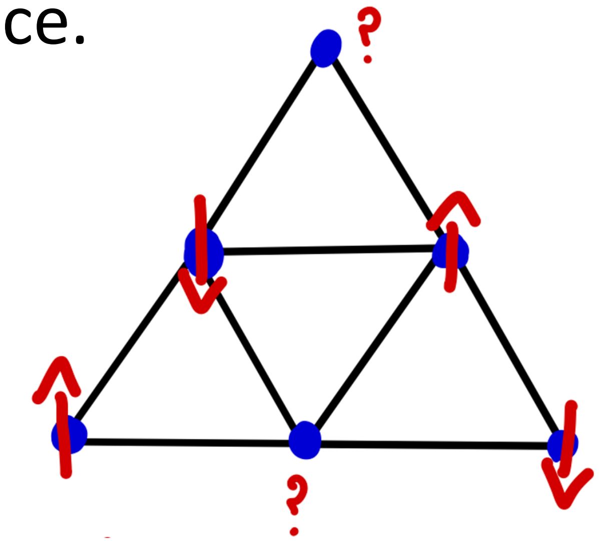


```
Spin Lattice:
 [[ 1 -1 -1]
 [-1  1  1]]

Total Energy (periodic boundary) : -6

Bit String:  [0 1 1 1 0 0]

Bit String Integer:  28
```

Next Step: Investigating Correlation

- Correlation refers to the macroscopic relationship between two specific dipoles in the system – essentially how the orientation of their spins relate to one another.

- By analyzing spin correlations, we can identify which dipoles are frustrated within the lattice.



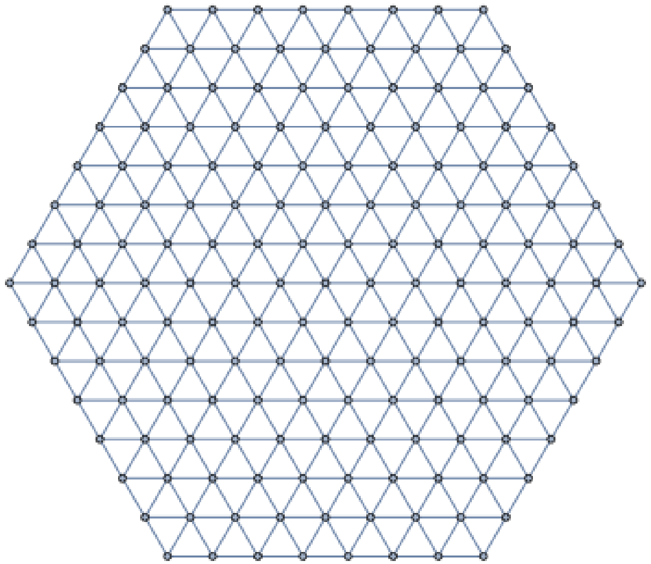


Figure 5: Finding which dipoles are frustrated is easy to identify on a smaller lattice, but is much more complex when the lattice becomes larger. [4]

Finding Correlation using Pauli Matrices

- To find the correlation between two specific dipoles, we need to do some math to calculate the "magnetic moment" of the system, (i.e., the expectation value of the spins)
  - To do this, we can use Pauli's spin operators – specifically the σ_z operator.

$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$\sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Example:

- Suppose a pair of dipoles exist in a superposition of 3 different states:
  - up-up, down-down, and up-down

- We can represent this as: $|\psi> = \frac{1}{\sqrt{3}}[\,|\uparrow\uparrow> \; + \; |\downarrow\downarrow> \; +|\uparrow\downarrow>]$

$$|\uparrow\uparrow> = \begin{bmatrix}1\\0\end{bmatrix} \otimes \begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1\\0\\0\\0\end{bmatrix} \quad |\downarrow\downarrow> = \begin{bmatrix}0\\1\end{bmatrix} \otimes \begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\0\\0\\1\end{bmatrix} \quad |\uparrow\downarrow> = \begin{bmatrix}1\\0\end{bmatrix} \otimes \begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$

$$\therefore |\psi> = \frac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\0\\1\end{bmatrix}$$

- Now, we can apply the Pauli Matrices as follows, and after some matrix multiplication, we can find the correlation between the two spins:

$$< \psi\, |\sigma_z \otimes \sigma_z|\, \psi > = \frac{1}{3}\begin{bmatrix}1 & 1 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}\begin{bmatrix}1\\ 1\\ 0\\ 1\end{bmatrix}$$

$$= \frac{1}{3}\begin{bmatrix}1 & 1 & 0 & 1\end{bmatrix}\begin{bmatrix}1\\ -1\\ 0\\ 1\end{bmatrix}$$

$$= \frac{1}{3}$$

Adding in more dipoles

- Now that we have a way of comparing two dipoles directly, we need to find a way to analyze a system with many dipoles.

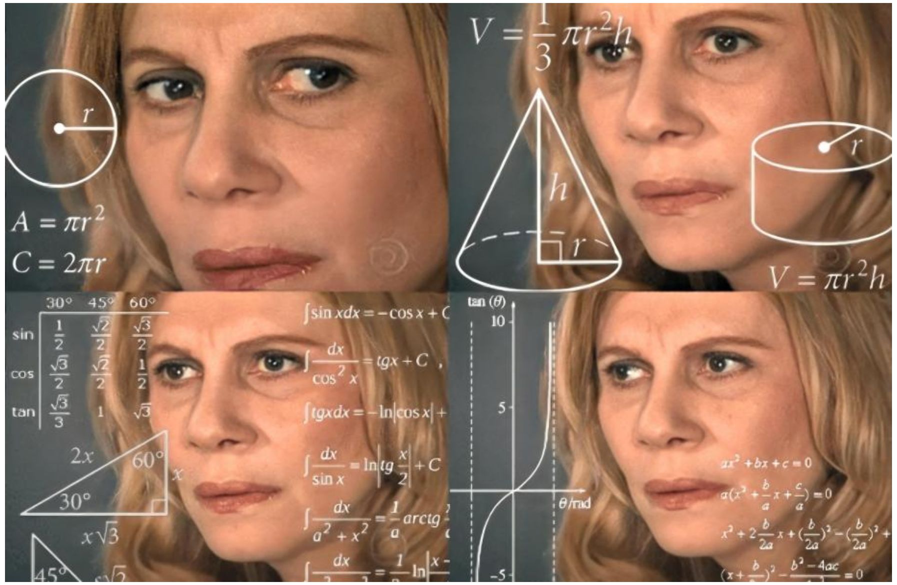
- Specifically, we need to be able to analyze the interactions between any specific pair of dipoles. We can do this with modification to our wavefunction with the introduction of identity matrices:

$$< \psi \mid \sigma_z \otimes \sigma_z \otimes I_1 \otimes I_2 \otimes \cdots \otimes I_n \mid \psi >$$

Too Many Tensors…

- The problem I quickly encountered with this approach was that the Kronecker products rapidly became exponentially large, which was not only difficult to wrap my mind around but would also be very computationally expensive.

- I needed to find a new approach that worked better for computational tools…



Shifting to a Probabilistic Approach

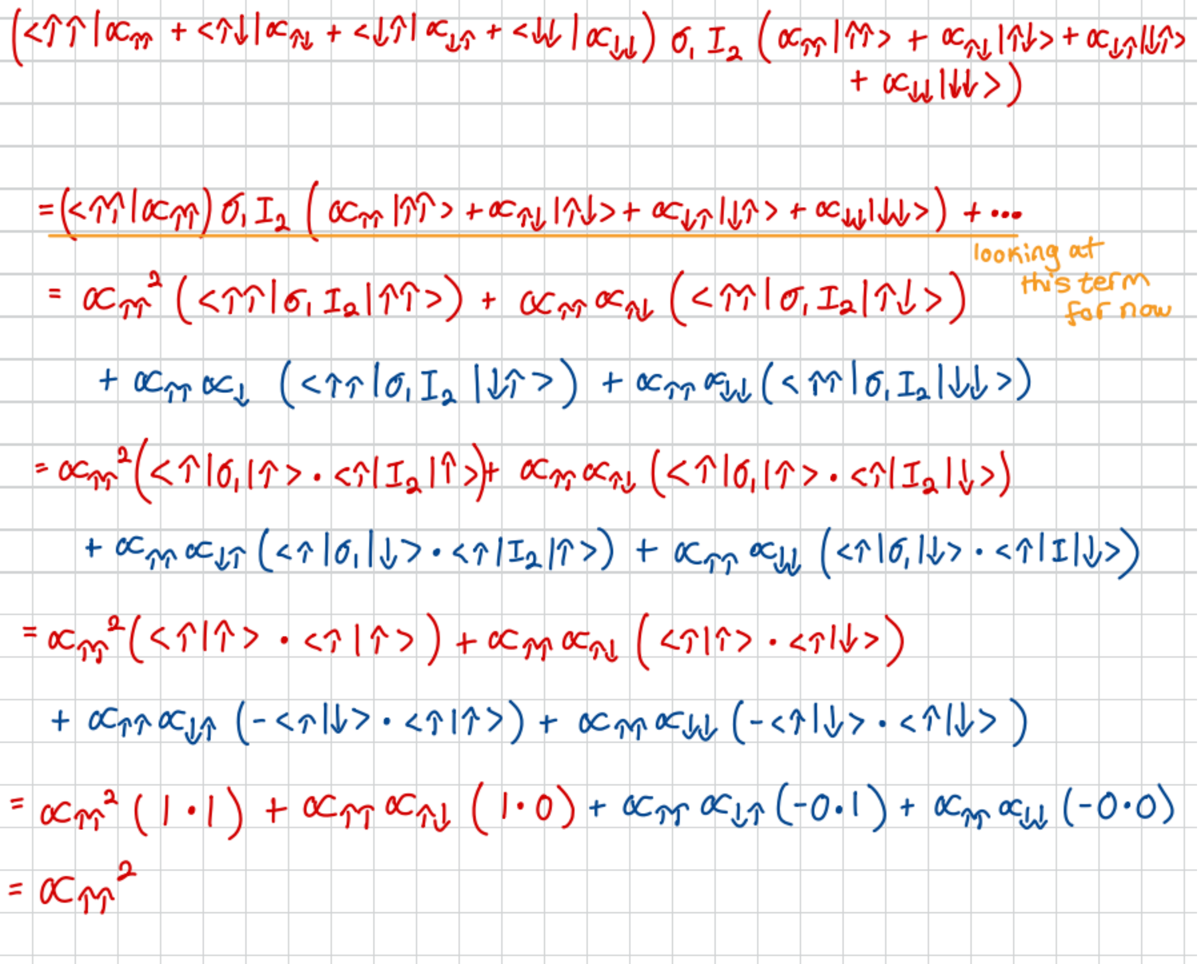
- Shifting the way we approached the problem; we can look at the probabilities of each configuration occurring and use those to quickly compute $| \psi >$

- If we define the state to be the following: $|\psi\rangle = \sum_{i\in\{0,1\}} \sum_{j\in\{0,1\}} \alpha_{ij} |ij\rangle$

- Then when we analyze the following: $\langle\psi| \sigma_z \otimes \ I_2 |\psi\rangle$

- We get a ton of Math!

A lot of work by hand…



$$\left(\langle\uparrow\uparrow|\alpha_{\uparrow\uparrow} + \langle\uparrow\downarrow|\alpha_{\uparrow\downarrow} + \langle\downarrow\uparrow|\alpha_{\downarrow\uparrow} + \langle\downarrow\downarrow|\alpha_{\downarrow\downarrow}\right)\sigma_1 I_2 \left(\alpha_{\uparrow\uparrow}|\uparrow\uparrow\rangle + \alpha_{\uparrow\downarrow}|\uparrow\downarrow\rangle + \alpha_{\downarrow\uparrow}|\downarrow\uparrow\rangle + \alpha_{\downarrow\downarrow}|\downarrow\downarrow\rangle\right)$$

$$= \underline{\left(\langle\uparrow\uparrow|\alpha_{\uparrow\uparrow}\right)\sigma_1 I_2 \left(\alpha_{\uparrow\uparrow}|\uparrow\uparrow\rangle + \alpha_{\uparrow\downarrow}|\uparrow\downarrow\rangle + \alpha_{\downarrow\uparrow}|\downarrow\uparrow\rangle + \alpha_{\downarrow\downarrow}|\downarrow\downarrow\rangle\right) + \dots}$$

looking at this term for now

$$= \alpha_{\uparrow\uparrow}^2\left(\langle\uparrow\uparrow|\sigma_1 I_2|\uparrow\uparrow\rangle\right) + \alpha_{\uparrow\uparrow}\alpha_{\uparrow\downarrow}\left(\langle\uparrow\uparrow|\sigma_1 I_2|\uparrow\downarrow\rangle\right)$$

$$+ \alpha_{\uparrow\uparrow}\alpha_{\downarrow}\left(\langle\uparrow\uparrow|\sigma_1 I_2|\downarrow\uparrow\rangle\right) + \alpha_{\uparrow\uparrow}\alpha_{\downarrow\downarrow}\left(\langle\uparrow\uparrow|\sigma_1 I_2|\downarrow\downarrow\rangle\right)$$

$$= \alpha_{\uparrow\uparrow}^2\left(\langle\uparrow|\sigma_1|\uparrow\rangle \cdot \langle\uparrow|I_2|\uparrow\rangle\right) + \alpha_{\uparrow\uparrow}\alpha_{\uparrow\downarrow}\left(\langle\uparrow|\sigma_1|\uparrow\rangle \cdot \langle\uparrow|I_2|\downarrow\rangle\right)$$

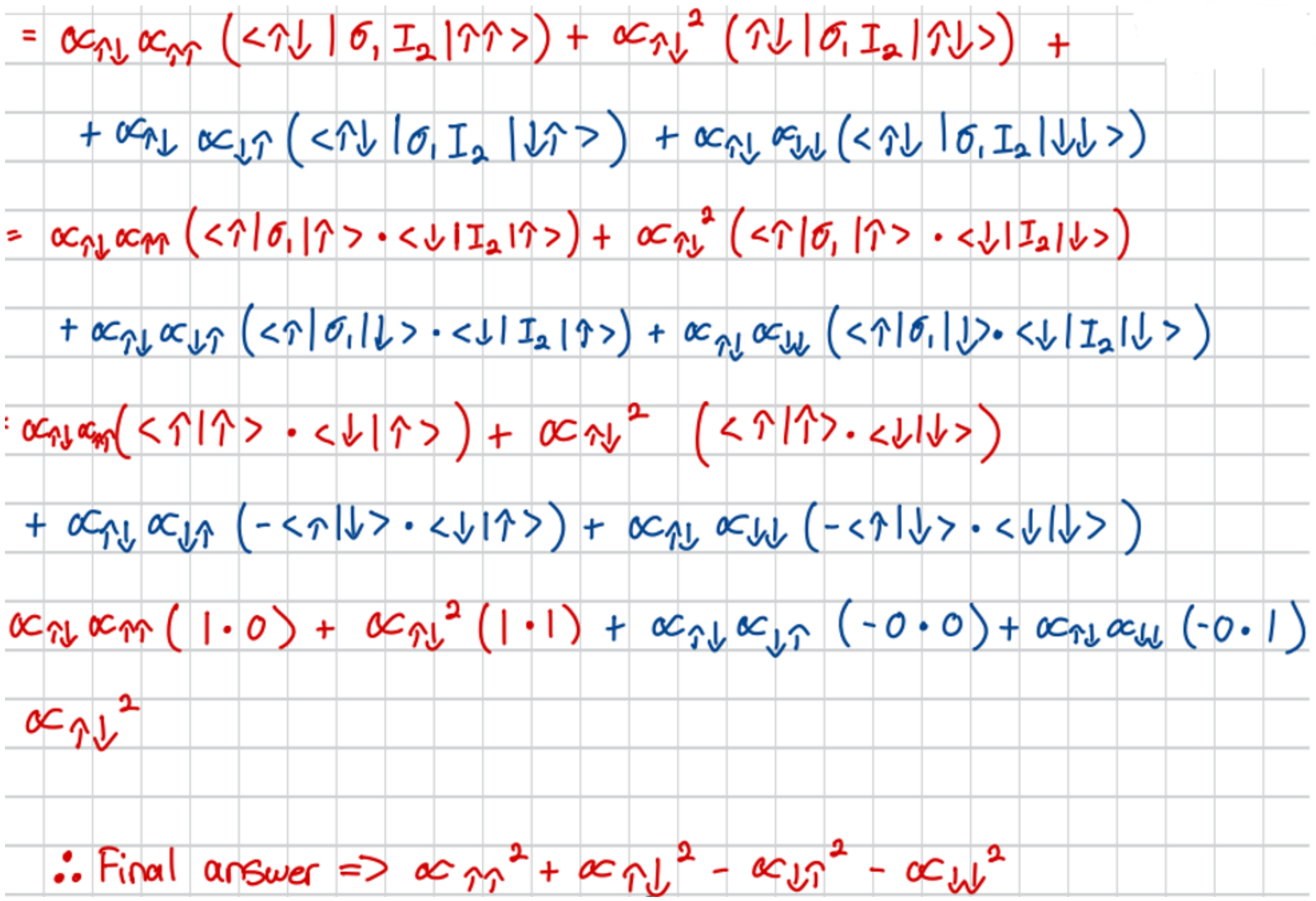
$$+ \alpha_{\uparrow\uparrow}\alpha_{\downarrow\uparrow}\left(\langle\uparrow|\sigma_1|\downarrow\rangle \cdot \langle\uparrow|I_2|\uparrow\rangle\right) + \alpha_{\uparrow\uparrow}\alpha_{\downarrow\downarrow}\left(\langle\uparrow|\sigma_1|\downarrow\rangle \cdot \langle\uparrow|I|\downarrow\rangle\right)$$

$$= \alpha_{\uparrow\uparrow}^2\left(\langle\uparrow|\uparrow\rangle \cdot \langle\uparrow|\uparrow\rangle\right) + \alpha_{\uparrow\uparrow}\alpha_{\uparrow\downarrow}\left(\langle\uparrow|\uparrow\rangle \cdot \langle\uparrow|\downarrow\rangle\right)$$

$$+ \alpha_{\uparrow\uparrow}\alpha_{\downarrow\uparrow}\left(-\langle\uparrow|\downarrow\rangle \cdot \langle\uparrow|\uparrow\rangle\right) + \alpha_{\uparrow\uparrow}\alpha_{\downarrow\downarrow}\left(-\langle\uparrow|\downarrow\rangle \cdot \langle\uparrow|\downarrow\rangle\right)$$

$$= \alpha_{\uparrow\uparrow}^2(1\cdot 1) + \alpha_{\uparrow\uparrow}\alpha_{\uparrow\downarrow}(1\cdot 0) + \alpha_{\uparrow\uparrow}\alpha_{\downarrow\uparrow}(-0\cdot 1) + \alpha_{\uparrow\uparrow}\alpha_{\downarrow\downarrow}(-0\cdot 0)$$

$$= \alpha_{\uparrow\uparrow}^2$$



$$= \alpha_{\uparrow\downarrow}\alpha_{\uparrow\uparrow}\left(\langle\uparrow\downarrow|\sigma_1 I_2|\uparrow\uparrow\rangle\right) + \alpha_{\uparrow\downarrow}^2\left(\uparrow\downarrow|\sigma_1 I_2|\uparrow\downarrow\rangle\right) +$$

$$+ \alpha_{\uparrow\downarrow}\alpha_{\downarrow\uparrow}\left(\langle\uparrow\downarrow|\sigma_1 I_2|\downarrow\uparrow\rangle\right) + \alpha_{\uparrow\downarrow}\alpha_{\downarrow\downarrow}\left(\langle\uparrow\downarrow|\sigma_1 I_2|\downarrow\downarrow\rangle\right)$$

$$= \alpha_{\uparrow\downarrow}\alpha_{\uparrow\uparrow}\left(\langle\uparrow|\sigma_1|\uparrow\rangle \cdot \langle\downarrow|I_2|\uparrow\rangle\right) + \alpha_{\uparrow\downarrow}^2\left(\langle\uparrow|\sigma_1|\uparrow\rangle \cdot \langle\downarrow|I_2|\downarrow\rangle\right)$$

$$+ \alpha_{\uparrow\downarrow}\alpha_{\downarrow\uparrow}\left(\langle\uparrow|\sigma_1|\downarrow\rangle \cdot \langle\downarrow|I_2|\uparrow\rangle\right) + \alpha_{\uparrow\downarrow}\alpha_{\downarrow\downarrow}\left(\langle\uparrow|\sigma_1|\downarrow\rangle \cdot \langle\downarrow|I_2|\downarrow\rangle\right)$$

$$= \alpha_{\uparrow\downarrow}\alpha_{\uparrow\uparrow}\left(\langle\uparrow|\uparrow\rangle \cdot \langle\downarrow|\uparrow\rangle\right) + \alpha_{\uparrow\downarrow}^2\left(\langle\uparrow|\uparrow\rangle \cdot \langle\downarrow|\downarrow\rangle\right)$$

$$+ \alpha_{\uparrow\downarrow}\alpha_{\downarrow\uparrow}\left(-\langle\uparrow|\downarrow\rangle \cdot \langle\downarrow|\uparrow\rangle\right) + \alpha_{\uparrow\downarrow}\alpha_{\downarrow\downarrow}\left(-\langle\uparrow|\downarrow\rangle \cdot \langle\downarrow|\downarrow\rangle\right)$$

$$\alpha_{\uparrow\downarrow}\alpha_{\uparrow\uparrow}(1\cdot 0) + \alpha_{\uparrow\downarrow}^2(1\cdot 1) + \alpha_{\uparrow\downarrow}\alpha_{\downarrow\uparrow}(-0\cdot 0) + \alpha_{\uparrow\downarrow}\alpha_{\downarrow\downarrow}(-0\cdot 1)$$

$$\alpha_{\uparrow\downarrow}^2$$

$\therefore$ Final answer $\Rightarrow \alpha_{\uparrow\uparrow}^2 + \alpha_{\uparrow\downarrow}^2 - \alpha_{\downarrow\uparrow}^2 - \alpha_{\downarrow\downarrow}^2$

Less Work by hand…

- Simplified Series solution to the previous slide:

$$\langle\psi|\sigma_z I|\psi\rangle = \sum_{i',j'\in\{0,1\}}\sum_{i,j\in\{0,1\}} \alpha_{i'j'}\,\alpha_{ij}\,\langle i'j'|\sigma_z I|ij\rangle$$

$$= \sum\sum \alpha_{i'j'}\,\alpha_{ij}\,(-1)^{i}\,\underbrace{\langle i'|i\rangle}_{\delta_{i'i}}\cdot\underbrace{\langle j'|j\rangle}_{\delta_{j'j}}$$

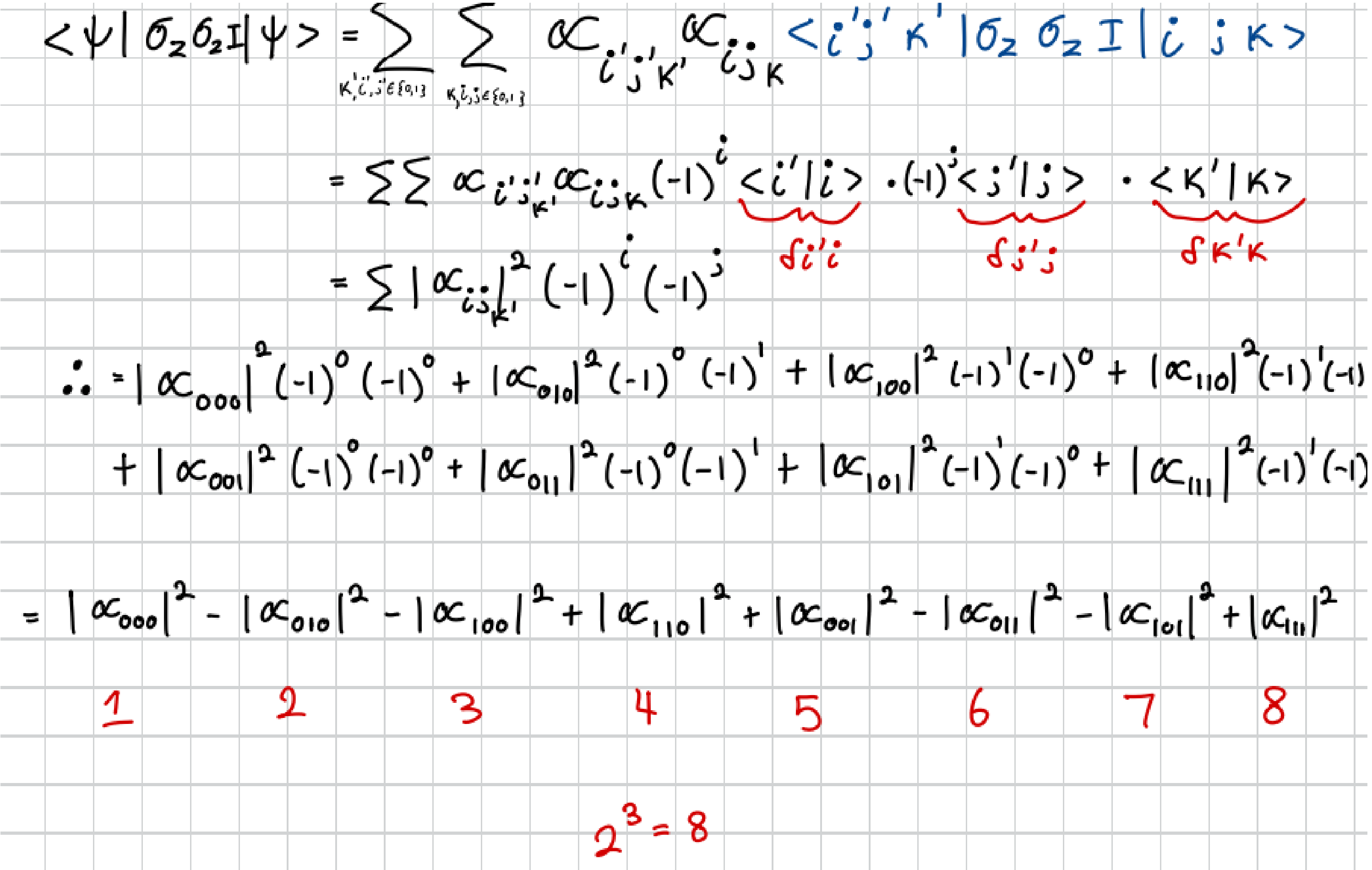
$$= \sum|\alpha_{ij}|^2(-1)^{i}$$

$$\therefore = |\alpha_{00}|^2(-1)^0 + |\alpha_{01}|^2(-1)^0 + |\alpha_{10}|^2(-1)^1 + |\alpha_{11}|^2(-1)^2$$

$$= |\alpha_{00}|^2 + |\alpha_{01}|^2 - |\alpha_{10}|^2 - |\alpha_{11}|^2$$

Expanding the Solution

- Now, we can expand the previous solution to a 3-dipole system:



$$\langle\psi|\sigma_z\sigma_z I|\psi\rangle = \sum_{k',i',j'\in\{0,1\}}\ \sum_{k,i,j\in\{0,1\}} \alpha_{i'j'k'}\alpha_{ijk} \langle i'j'k'|\sigma_z\,\sigma_z\, I|i\,j\,k\rangle$$

$$= \sum\sum \alpha_{i'j'k'}\alpha_{ijk}(-1)^{i}\underbrace{\langle i'|i\rangle}_{\delta_{i'i}}\cdot(-1)^{j}\underbrace{\langle j'|j\rangle}_{\delta_{j'j}}\cdot\underbrace{\langle k'|k\rangle}_{\delta_{k'k}}$$

$$= \sum|\alpha_{ijk'}|^2(-1)^{i}(-1)^{j}$$

$$\therefore = |\alpha_{000}|^2(-1)^0(-1)^0 + |\alpha_{010}|^2(-1)^0(-1)^1 + |\alpha_{100}|^2(-1)^1(-1)^0 + |\alpha_{110}|^2(-1)^1(-1$$

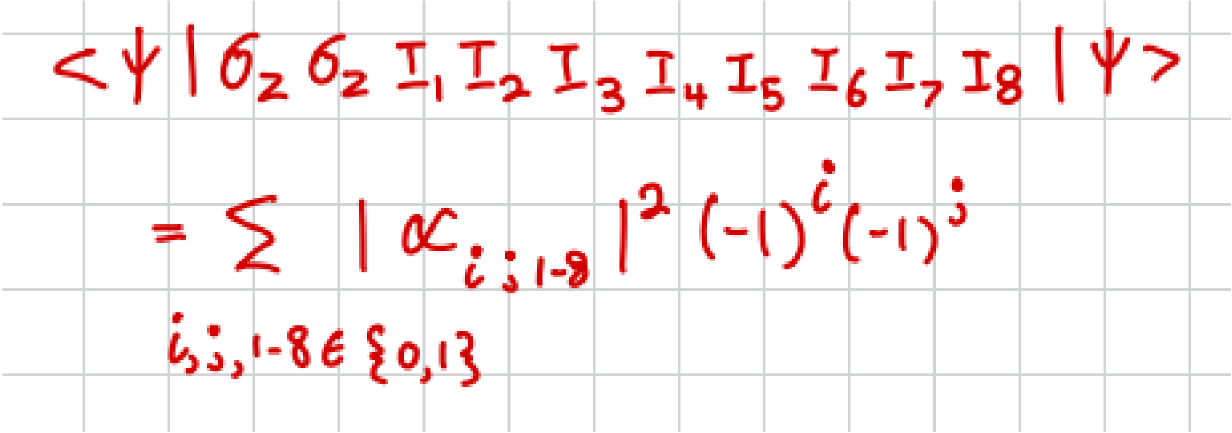
$$+ |\alpha_{001}|^2(-1)^0(-1)^0 + |\alpha_{011}|^2(-1)^0(-1)^1 + |\alpha_{101}|^2(-1)^1(-1)^0 + |\alpha_{111}|^2(-1)^1(-1)$$

$$= \underset{1}{|\alpha_{000}|^2} - \underset{2}{|\alpha_{010}|^2} - \underset{3}{|\alpha_{100}|^2} + \underset{4}{|\alpha_{110}|^2} + \underset{5}{|\alpha_{001}|^2} - \underset{6}{|\alpha_{011}|^2} - \underset{7}{|\alpha_{101}|^2} + \underset{8}{|\alpha_{111}|^2}$$

$$2^3 = 8$$

Expanding the Solution

- And this method works with n-dipole systems! And we only need to keep track of the spins of whatever dipoles we specify “i” and “j” to be:

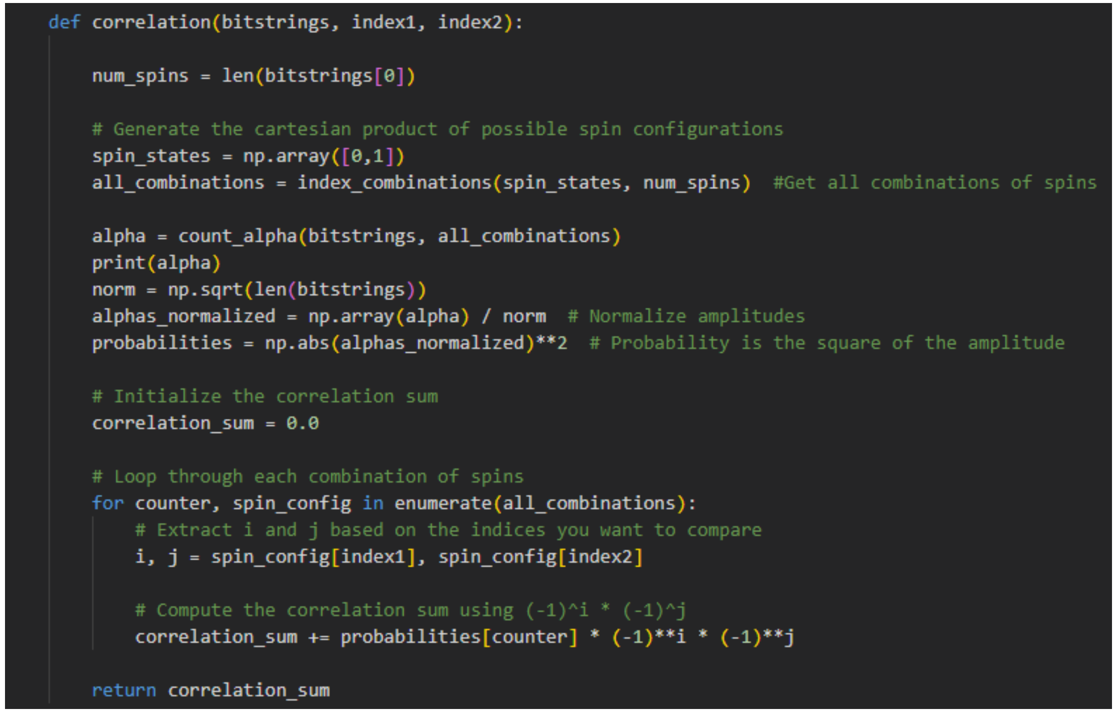


$$\langle\psi|\sigma_z\sigma_z I_1 I_2 I_3 I_4 I_5 I_6 I_7 I_8|\psi\rangle$$

$$= \sum_{i,j,1\text{-}8\in\{0,1\}} |\alpha_{i\,j\,1\text{-}8}|^2(-1)^i(-1)^j$$

Applying all this Math to the Simulation

- Now that we have a much simpler way to find the correlation between two dipoles, we can analyze how frequently each configuration occurred and sum up all the terms to get a final expectation value.



```python
def correlation(bitstrings, index1, index2):

    num_spins = len(bitstrings[0])

    # Generate the cartesian product of possible spin configurations
    spin_states = np.array([0,1])
    all_combinations = index_combinations(spin_states, num_spins)  #Get all combinations of spins

    alpha = count_alpha(bitstrings, all_combinations)
    print(alpha)
    norm = np.sqrt(len(bitstrings))
    alphas_normalized = np.array(alpha) / norm  # Normalize amplitudes
    probabilities = np.abs(alphas_normalized)**2  # Probability is the square of the amplitude

    # Initialize the correlation sum
    correlation_sum = 0.0

    # Loop through each combination of spins
    for counter, spin_config in enumerate(all_combinations):
        # Extract i and j based on the indices you want to compare
        i, j = spin_config[index1], spin_config[index2]

        # Compute the correlation sum using (-1)^i * (-1)^j
        correlation_sum += probabilities[counter] * (-1)**i * (-1)**j

    return correlation_sum
```

The Program Works! Well, in a limited way…

- It works well for small lattices! I was able to find the correlations between any specified dipole that matches the expected results if we do the calculation by hand, the Kronecker Product way.

- However, even with simplified probabilistic calculation, this is very computationally expensive due to the exponential nature of possible configurations.
  - Program struggles to analyze lattices greater then 4x4.

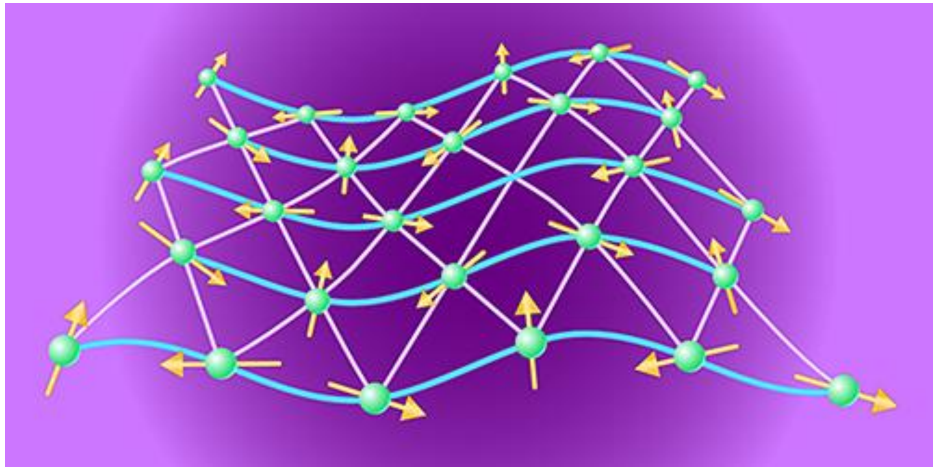


Figure 6: 3D rendering of a triangular lattice with interacting dipoles. [5]

How to Move Forward From Here

- The next steps for this project would involve:
  - creating models that explore results of correlation further
  - finding ways to visualize this data
  - and overall, open the door to begin asking questions about what variables we can manipulate and observe how the system behaves as a result

- Unfortunately, I was not able to get to the point where I would be able to make these next steps, as I just finished debugging the program and getting every small component to work as intended and I ran out of time…
  - But the foundation to begin moving forward and asking those questions is complete!

Literature Survey

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Thank you for your time!

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